

# On the Non-Relativistic Groundstate Energy of Positronium in Relativistic Schrödinger Theory

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## Abstract

The *Relativistic Schrödinger Theory* (RST) has been set up as an alternative form of particle theory. This theory obeys the fundamental symmetries which are required to hold for any meaningful theory: gauge and Lorentz covariance (RST can be formulated even over a pseudo-Riemannian space-time). But the question is now whether obeying those fundamental symmetries is sufficient for the practical success of a theory, i.e. whether the predictions are in agreement with the experimental findings. In this context, the non-relativistic energy spectrum of positronium has been considered in some precedent papers. Here, the problem is that exact solutions of the RST eigenvalue system cannot be obtained and one has to resort to approximate solutions. For this purpose, a variational method is applied in the present paper which yields the RST groundstate energy smaller than the former results and than its conventional counterpart by some 10%. Such deviations are also observed when one compares the approximate RST spectrum (up to quantum numbers  $n \approx 100$ ) to the corresponding predictions of the conventional theory. It seems presently not possible to decide whether those deviations are due to RST itself or are merely due to the applied approximation technique. Thus the practical usefulness of RST must remain unclarified for the moment.

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## 1. *RST Eigenvalue Problem*

In conventional quantum mechanics, the internal energy spectrum of non-relativistic positronium is obtained by solving the linear two-particle eigenvalue problem

$$\hat{H}_{\mathcal{P}} |\Phi_n\rangle = E_{\text{conv}}^{(n)} |\Phi_n\rangle \quad (1)$$

due to the positronium Hamiltonian  $\hat{H}_{\mathcal{P}}$

$$\hat{H}_{\mathcal{P}} = -\frac{\hbar^2}{M} \Delta - \frac{e^2}{r} . \quad (2)$$

Such a linear eigenvalue problem can easily be solved exactly, and the resulting energy spectrum  $E_{\text{conv}}^{(n)}$  looks as follows [1]

$$E_{\text{conv}}^{(n)} = -\frac{e^2}{4a_B} \cdot \frac{1}{n^2} . \quad (3)$$

$$\left( \frac{e^2}{4a_B} \simeq 6,8029 \dots \text{ [eV]} \right)$$

This conventional spectrum ( $n = 1, 2, 3, 4, \dots$ ) is relatively close to the experimental finding. The remaining experimental deviations from the theoretical predictions (3) are usually traced back to the neglected magnetic and relativistic effects [2]. Thus the picture of positronium appears quite convincing within the framework of conventional quantum theory which itself is conceived as a *probabilistic point-particle* theory.

However, the observational data do support sometimes also a *fluid-dynamic* picture of the quantum events so that one is forced to resort to the notorious particle-wave duality [3]. If one wishes to take this kind of duality in earnest, one should feel forced oneself to elaborate the fluid-dynamic aspects of the quantum events to a degree being comparable to the point-particle approach. An attempt pointing in this direction has been undertaken in form of the *Relativistic Schrödinger Theory* (see ref. [4] and the references cited therein). In the present context of the positronium spectrum, the main difference between RST and the conventional theory concerns the treatment of the electromagnetic interactions between both particles (i.e. electron and positron). Here, the conventional

point-particle theory relies on the *fixed* Coulomb potential (see equation (2)) and thus does not equip the electric interaction field with a proper dynamical degree of freedom. Therefore the conventional theory deals only with the matter field  $\Phi(\vec{r})$  as a dynamical variable (see equation (1)) but does not take into account a similar field equation for the electric interaction potential ( $A(\vec{r})$ , say).

In contrast to such a truncating approach, RST adopts the electric interaction field as a truly dynamical constituent of the two-particle system and therefore equips the electric potential  $A(\vec{r})$  with a field equation of its own, namely the Poisson equation, i.e. for the present static situation

$$\Delta A(r) = -\frac{\alpha_s}{r} (\Phi(r))^2 . \quad (4)$$

Here, the wave function  $\Phi(r)$  acts as the source of the electrostatic potential  $A(r)$  and obeys itself a Schrödinger-like eigenvalue equation

$$-\frac{\hbar^2}{2M} \left( \frac{d^2 \Phi(r)}{dr^2} + \frac{1}{r} \frac{d \Phi(r)}{dr} \right) + \frac{\hbar^2 \ell_{\mathcal{P}}^2}{2Mr^2} \cdot \Phi(r) - \hbar c A(r) \cdot \Phi(r) = E_* \cdot \Phi(r) \quad (5)$$

(for the deduction of these spherically symmetric equations from the general RST dynamics see ref. [4]). For the purpose of inspecting the groundstate one puts for the principal quantum number  $n_{\mathcal{P}} (\doteq \ell_{\mathcal{P}} + 1) = 1$  which somewhat simplifies the matter equation (5).

But the price for including the electric interaction potential  $A(r)$  (as a dynamical quantity on the same footing as the matter field  $\Phi(r)$ ) is a considerable complication which prevents one from finding exact solutions of that non-linear eigenvalue problem (4)-(5). Nevertheless one would like to get at least a rough idea of what kind of energy spectrum does arise from that eigenvalue problem (4)-(5). Here, one possibility is to exploit the fact that those eigenvalue equations can be conceived as the minimal equations due to a certain functional, i.e. the RST energy functional  $\mathbb{E}_{\text{RST}}$ , see equation (8) below. This suggests to apply some variational technique for calculating the desired energy spectrum. Especially for the groundstate one can consider trial functions for the matter field  $\Phi(r)$  and the interaction potential  $A(r)$  in order to substitute both in the energy functional  $\mathbb{E}_{\text{RST}}$

which thus becomes a function of the variational parameters contained in the trial ansatz for  $\Phi(r)$  and  $A(r)$ . In the last step one looks for the minimal value,  $\mathbb{E}_\infty^{[0]}$  say, of the energy function with respect to the variational parameters and thus obtains a first estimate of the groundstate energy.

Such an estimate should be sufficient in order to see whether (or not) the RST energy spectrum can be close to the conventional spectrum  $E_{\text{conv}}^{(n)}$  (3). Namely, supposing that the RST energy functional  $\mathbb{E}_{\text{RST}}$  is bounded from below ( $\leadsto$  finite ground-state energy  $\mathbb{E}_{\text{RST}}^{[0]}$ ), that approximate groundstate energy  $\mathbb{E}_\infty^{[0]}$  (obtained by means of the variational method) must be *higher* than the *exact* but unknown RST groundstate energy  $\mathbb{E}_{\text{RST}}^{[0]}$ , i.e.  $\mathbb{E}_\infty^{[0]} > \mathbb{E}_{\text{RST}}^{[0]}$ . If now the *approximate* energy  $\mathbb{E}_\infty^{[0]}$  turns out to be essentially smaller than the conventional counterpart  $E_{\text{conv}}^{(1)} = -6.8029$  [eV], i.e.  $\mathbb{E}_\infty^{[0]} < E_{\text{conv}}^{(1)}$ , then we have to conclude that the *exact* RST groundstate energy  $\mathbb{E}_{\text{RST}}^{[0]}$  is even farer away from its conventional counterpart:  $\mathbb{E}_{\text{RST}}^{[0]} \ll E_{\text{conv}}^{(1)}$ ; and this then says that the present RST cannot be considered a serious competitor of the conventional theory, at least as far as the positronium groundstate is concerned. Regrettably, this is the outcome of the present investigation: by means of a certain variational ansatz  $\Psi_\infty^{\{0\}}(y)$ , see equation (40) below, the corresponding groundstate energy  $\mathbb{E}_\infty^{[0]}$  is found as  $-7,6644 \dots$  [eV] in place of the conventional  $E_{\text{conv}}^{(1)} = -6,8029$  [eV] (3), see **Fig.2** below.

The conclusion is that either RST itself is unapt or the present spherically symmetric approximation, as described below (IV.5a)-(IV.5d) of ref. [4], is inadequate. In the latter case it seems worthwhile to think about a more adequate version of spherically symmetric approximation in RST. The present result for the whole energy spectrum, see **table II** below, seems to provide sufficient motivation for such an endeavour.

## 2. Principle of Minimal Energy

The present RST eigenvalue system (4)–(5) is evidently of non-linear character because the potential  $A(r)$  in the Schrödinger-like equation (5) for the wave function  $\Phi(r)$  is

determined by the wave function  $\Phi(r)$  itself, see the Poisson equation (4). It should be a matter of course that such a non-linear eigenvalue system, as constituted by the equations (4)–(5), is much more difficult to solve than its conventional counterpart (1); and an exact solution of (4)–(5) is presently not known so that one has to be satisfied with approximate solutions. Here, a fortunate circumstance is of great help. Namely, the system (4)–(5) represents the extremal equations due to a certain energy functional ( $\mathbb{E}_{\text{RST}}[\Phi, A]$ , say). More concretely, the Poisson equation (4) emerges as the Euler-Lagrange equation for extremalizing the energy functional  $\mathbb{E}_{\text{RST}}$  with respect to the electrostatic potential  $A$

$$\frac{\delta \mathbb{E}_{\text{RST}}[\Phi, A]}{\delta A} = 0 , \quad (6)$$

and similarly the eigenvalue equation (5) may be considered the extremal equation with respect to the matter field  $\Phi$ :

$$\frac{\delta \mathbb{E}_{\text{RST}}[\Phi, A]}{\delta \Phi} = 0 . \quad (7)$$

Here the energy functional  $\mathbb{E}_{\text{RST}}[\Phi, A]$  principally looks as follows

$$\mathbb{E}_{\text{RST}} = \mathbb{E}_{\text{RST}}^{(\text{G})} + \mathbb{E}_{\text{RST}}^{(\text{D})} . \quad (8)$$

This says that the total energy  $\mathbb{E}_{\text{RST}}$  is the sum of the gauge-field energy  $\mathbb{E}_{\text{RST}}^{(\text{G})}$  and the energy  $\mathbb{E}_{\text{RST}}^{(\text{D})}$  being concentrated in the Dirac matter field. In the non-relativistic electrostatic approximation, the gauge-field energy  $\mathbb{E}_{\text{RST}}^{(\text{G})}$  becomes simplified to the generalized electrostatic field energy  $\mathbb{E}_{\text{RST}}^{[\text{e}]}$ , i. e.

$$\mathbb{E}_{\text{RST}}^{(\text{G})} \Rightarrow \mathbb{E}_{\text{RST}}^{[\text{e}]} = \mathbb{E}_{\text{R}}^{[\text{e}]} + \lambda_{\text{G}}^{(\text{e})} \cdot \mathbb{N}_{\text{G}}^{[\text{e}]} . \quad (9)$$

Here, the first part  $\mathbb{E}_{\text{R}}^{[\text{e}]}$  is the usual electrostatic field energy

$$\mathbb{E}_{\text{R}}^{[\text{e}]} = -\frac{\hbar c}{\alpha_{\text{s}}} \int_0^\infty dr r^2 \left( \frac{d A(r)}{dr} \right)^2 , \quad (10)$$

$\lambda_{\text{G}}^{(\text{e})}$  is a Lagrangean multiplier ( $\lambda_{\text{G}}^{(\text{e})} = -2$ ) which is due to the Poisson constraint  $\mathbb{N}_{\text{G}}^{[\text{e}]}$ , measuring the deviation of the electrostatic field energy  $\mathbb{E}_{\text{R}}^{[\text{e}]}$  (10) from its “mass equivalent”

$$\mathbb{M}^{[e]} c^2$$

$$\mathbb{M}^{[e]} c^2 \doteq -\hbar c \int_0^\infty dr r A(r) \cdot (\Phi(r))^2 , \quad (11)$$

i. e.

$$\mathbb{N}_G^{[e]} \doteq \mathbb{E}_R^{[e]} - \mathbb{M}^{[e]} c^2 . \quad (12)$$

One can easily show (by means of the Poisson equation (4)) that the Poisson constraint  $\mathbb{N}_G^{[e]}$  vanishes whenever the potential  $A(r)$  is an *exact* solution of that Poisson equation (4).

The second constituent  $\mathbb{E}_{\text{RST}}^{(\text{D})}$  of the energy functional  $\mathbb{E}_{\text{RST}}$  (8) measures the energy being located in the Dirac matter field. In the non-relativistic approximation, the Dirac four-spinor degenerates to a simple scalar field  $\Phi(r)$  which then essentially carries the non-relativistic matter energy  $\mathbb{E}_D$

$$E_{\text{RST}}^{(\text{D})} \Rightarrow \mathbb{E}_D + \lambda_D \cdot \mathbb{N}_D . \quad (13)$$

Here, the proper matter energy  $\mathbb{E}_D$  (in a state with quantum number  $\ell_{\mathcal{P}}$ ) is defined in terms of the non-relativistic scalar field  $\Phi$  through

$$\mathbb{E}_D^{\{\ell_{\mathcal{P}}\}} = \frac{\hbar^2}{M} \int_0^\infty dr r \left\{ \left( \frac{d\Phi(r)}{dr} \right)^2 + \ell_{\mathcal{P}}^2 \left( \frac{\Phi(r)}{r} \right)^2 \right\} , \quad (14)$$

and the second part  $\mathbb{N}_D$  is nothing else than the normalization condition on the non-relativistic scalar field  $\Phi(r)$ :

$$\mathbb{N}_D \doteq \int_0^\infty dr r (\Phi(r))^2 - 1 = 0 . \quad (15)$$

The Lagrangean multiplier  $\lambda_D$  turns out as the energy eigenvalue  $E_*$  ( $= -\lambda_D$ ) in equation (5). Observe also that the present normalization constraint (15) is necessary in order that the electrostatic potential  $A(r)$  adopts the standard Coulomb form at infinity ( $r \rightarrow \infty$ ). Indeed, the integral representation of the wanted solution  $A(r)$  of the Poisson equation (4) looks as follows

$$A(r) = \frac{\alpha_s}{4\pi} \int d^3\vec{r}' \frac{(\Phi(r'))^2}{r' \cdot \|\vec{r} - \vec{r}'\|} . \quad (16)$$

Thus, the behaviour of this potential at infinity ( $r \rightarrow \infty$ ) actually is

$$\lim_{r \rightarrow \infty} A(r) = \frac{\alpha_s}{||\vec{r}||} \cdot \int_0^\infty dr' r' (\Phi(r'))^2 = \frac{\alpha_s}{r}, \quad (17)$$

just as a consequence of the normalization condition (15).

### 3. *Lowest-order Approximation of the Energy Spectrum*

An extremal principle is at hand now in form of the *principle of minimal energy*, cf. (6)–(7), which is assumed to associate a unique energy  $\mathbb{E}_{\text{RST}}^{[\ell_{\mathcal{P}}]}$  to any quantum number  $\ell_{\mathcal{P}}$ , namely by virtue of its minimal value on the space of trial fields  $A(r), \Phi(r)$ . This fortunate circumstance allows to approximately compute the energy spectrum  $\mathbb{E}_{\text{RST}}^{[\ell_{\mathcal{P}}]}$  where the quantum number  $\ell_{\mathcal{P}}$  is to be defined as the principal quantum number  $n_{\mathcal{P}}$  minus one:  $\ell_{\mathcal{P}} \doteq n_{\mathcal{P}} - 1$ . The computation of the whole spectrum  $\mathbb{E}_{\text{RST}}^{[\ell_{\mathcal{P}}]}$  ( $\ell_{\mathcal{P}} = 0, 1, 2, 3, \dots$ ) will first be presented in lowest approximation order and afterwards we concentrate on the ground-state energy  $\mathbb{E}_{\text{RST}}^{[0]}$ , i. e.  $\ell_{\mathcal{P}} = \mathbf{0}$ , because thereby does occur a certain curiosity. Namely, the *lowest-order* groundstate energy is found to coincide exactly with its conventional counterpart  $E_{\text{conv}}^{(1)}$  (3).

The groundstate energy (as that of any other excited energy state) may be estimated by *selecting* some plausible (normalized) wave function  $\Phi^{\{0\}}(r)$ , then substituting this trial ansatz on the right-hand side of the Poisson equation (4), in order to finally determine the associated gauge potential  $A^{\{0\}}(r)$ .

Since in this way both fields  $A^{\{0\}}(r)$  and  $\Phi^{\{0\}}(r)$  have been fixed, one can use these fields in order to determine the electrostatic field energy  $\mathbb{E}_{\text{R}}^{\{0\}}$  for the groundstate  $\ell_{\mathcal{P}} = \mathbf{0}$ , cf. (10)

$$\mathbb{E}_{\text{R}}^{[e]} \Big|_{\ell_{\mathcal{P}}=0} = \mathbb{E}_{\text{R}}^{\{0\}} \doteq -\frac{\hbar c}{\alpha_s} \int_0^\infty dr r^2 \left( \frac{d A^{\{0\}}(r)}{dr} \right)^2, \quad (18)$$



as well as the associated mass equivalent  $\mathbb{M}^{\{0\}}c^2$  (11)

$$\mathbb{M}^{\{0\}}c^2 = -\hbar c \int_0^\infty dr r A^{\{0\}}(r) \cdot (\Phi^{\{0\}}(r))^2. \quad (19)$$

The Poisson constraint  $\mathbb{N}_G^{[e]}$  for  $\ell_{\mathcal{P}} = 0$  (12) must be zero in this case ( $\mathbb{N}_{G,0}^{[e]} = 0$ ) because as trial potential  $A^{\{0\}}(r)$  an exact solution of the Poisson equation (4) is selected, i. e.

$$\Delta A^{\{0\}}(r) = -\frac{\alpha_s}{r} (\Phi^{\{0\}}(r))^2. \quad (20)$$

Furthermore, the trial wave function  $\Phi^{\{0\}}(r)$  is substituted in the matter-energy functional for the groundstate  $\mathbb{E}_D^{\{\ell_{\mathcal{P}}\}} (\ell_{\mathcal{P}} = 0: \mathbb{E}_D^{\{0\}})$

$$\mathbb{E}_D^{\{0\}} = \frac{\hbar^2}{M} \int_0^\infty dr r \cdot \left( \frac{d\Phi^{\{0\}}(r)}{dr} \right)^2, \quad (21)$$

so that now both constituents of the RST energy functional  $\mathbb{E}_{\text{RST}}^{\{\ell_{\mathcal{P}}\}}$  (8) (here  $\ell_{\mathcal{P}} = 0$ ) are fixed and the functional becomes an ordinary function of the trial parameters occurring in the selected trial ansatz  $\Phi^{\{0\}}(r)$ . The minimal value of this energy function over the trial-parameter space defines then the approximate groundstate energy  $\mathbb{E}^{[0]}$ . For the general situation with  $\ell_{\mathcal{P}} > 0$  one thus gets the spectrum  $\mathbb{E}^{[\ell_{\mathcal{P}}]}$ ,  $\ell_{\mathcal{P}} = n_{\mathcal{P}} - 1$ , with  $n_{\mathcal{P}}$  denoting the principal quantum number (of the hydrogen-like spectrum). It is true, the main concern of the present paper refers to the groundstate energy  $\mathbb{E}^{[0]}$ . However, for the sake of completeness we briefly discuss also the lowest-order approximations of the total spectrum.

The simplest example for the proposed procedure is based on the following (normalized, cf. (15)) trial amplitude  $\Phi_1^{\{\ell_{\mathcal{P}}\}}(r)$  [4]

$$\Phi_1^{\{\ell_{\mathcal{P}}\}}(r) = 2\beta \cdot \frac{(2\beta r)^{\ell_{\mathcal{P}}}}{\sqrt{(2\ell_{\mathcal{P}} + 1)!}} e^{-\beta r}, \quad (22)$$

where  $\beta$  is here the sole trial parameter. For this ansatz, the matter energy  $\mathbb{E}_{D,1}^{\{\ell_{\mathcal{P}}\}}$  (14) is

easily found to be of the form

$$\mathbb{E}_{\text{D},1}^{\{\ell_{\mathcal{P}}\}} = \varepsilon_{\text{kin},1}^{\{\ell_{\mathcal{P}}\}} \cdot \frac{e^2}{a_{\text{B}}} (2\beta a_{\text{B}})^2 = \frac{e^2}{4a_{\text{B}}} (2\beta a_{\text{B}})^2 \quad (23)$$

$$\left( a_{\text{B}} = \frac{\hbar^2}{M e^2} \dots \text{Bohr radius} \right) ,$$

and furthermore the associated solution  $A_1^{\{\ell_{\mathcal{P}}\}}(r)$  of the Poisson equation (4)

$$\Delta A_1^{\{\ell_{\mathcal{P}}\}}(r) = -\frac{\alpha_{\text{s}}}{r} \left( \Phi_1^{\{\ell_{\mathcal{P}}\}}(r) \right)^2 \quad (24)$$

is found as

$$A_1^{\{\ell_{\mathcal{P}}\}}(r) = \frac{\alpha_{\text{s}}}{r} (1 - e^{-2\beta r}) - 2\beta\alpha_{\text{s}} \frac{2\ell_{\mathcal{P}}}{1 + 2\ell_{\mathcal{P}}} \cdot e^{-2\beta r} . \quad (25)$$

$$\cdot \sum_{m=0}^{2\ell_{\mathcal{P}}-1} \frac{(2\beta r)^m}{m!} \left( 1 - \frac{2\ell_{\mathcal{P}} + 1}{2\ell_{\mathcal{P}}} \cdot \frac{m}{m+1} \right) .$$

This potential can now be used in order to calculate the electrostatic field energy  $E_{\text{R}}^{[\text{e}]}$  (10) which then appears for the present situation in the following form:

$$\mathbb{E}_{\text{R},1}^{\{\ell_{\mathcal{P}}\}} = -\frac{\hbar c}{\alpha_{\text{s}}} \int_0^\infty dr r^2 \left( \frac{d A_1^{\{\ell_{\mathcal{P}}\}}(r)}{dr} \right)^2 = -(2\beta a_{\text{B}}) \cdot \varepsilon_{\text{pot},1}^{\{\ell_{\mathcal{P}}\}} . \quad (26)$$

For specifying here the *potential coefficient*  $\varepsilon_{\text{pot},1}^{\{\ell_{\mathcal{P}}\}}$  it is very convenient to pass over to dimensionless objects  $y$ ,  $\mathcal{A}_1^{\{\ell_{\mathcal{P}}\}}(y)$ ,  $\Psi_1^{\{\ell_{\mathcal{P}}\}}(y)$  in the following way

$$y \doteq 2\beta r \quad (27\text{a})$$

$$\mathcal{A}_1^{\{\ell_{\mathcal{P}}\}}(y) \doteq \frac{1}{2\beta\alpha_{\text{s}}} A_1^{\{\ell_{\mathcal{P}}\}}(r) \quad (27\text{b})$$

$$\Psi_1^{\{\ell_{\mathcal{P}}\}}(y) \doteq \frac{\Phi_1^{\{\ell_{\mathcal{P}}\}}(r)}{2\beta} = \frac{1}{\sqrt{(2\ell_{\mathcal{P}} + 1)!}} y^{\ell_{\mathcal{P}}} e^{-y/2} . \quad (27\text{c})$$

This arrangement lets appear the potential coefficient as

$$\varepsilon_{\text{pot},1}^{\{\ell_{\mathcal{P}}\}} = \int_0^\infty dy y^2 \left( \frac{d \mathcal{A}_1^{\{\ell_{\mathcal{P}}\}}(y)}{dy} \right)^2 . \quad (28)$$

Substituting herein the calculated potential (25) yields

$$\varepsilon_{\text{pot},1}^{\{\ell_{\mathcal{P}}\}} = \frac{1}{2\ell_{\mathcal{P}}+1} \left\{ 1 + \frac{1}{(2\ell_{\mathcal{P}})!} \frac{1}{2^{2\ell_{\mathcal{P}}+1}} \left[ \frac{1}{2(2\ell_{\mathcal{P}}+1)} \sum_{n=0}^{2\ell_{\mathcal{P}}} \frac{(2\ell_{\mathcal{P}}+1+n)!}{2^n \cdot n!} - \sum_{n=0}^{2\ell_{\mathcal{P}}+1} \frac{(2\ell_{\mathcal{P}}+n)!}{2^n \cdot n!} \right] \right\}. \quad (29)$$

Alternatively, one could prefer to work also with the mass equivalent  $\mathbb{M}^{[\text{e}]}c^2$  (11) which for the present case appears as

$$\mathbb{M}_1^{\{\ell_{\mathcal{P}}\}}c^2 = -\hbar c \int_0^\infty dr r A_1^{\{\ell_{\mathcal{P}}\}}(r) \left( \Phi_1^{\{\ell_{\mathcal{P}}\}}(r) \right)^2 = -\frac{e^2}{a_B} (2\beta a_B) \cdot \mu_1^{\{\ell_{\mathcal{P}}\}} \quad (30)$$

with the *mass-equivalent coefficient*  $\mu_1^{\{\ell_{\mathcal{P}}\}}$  being defined through

$$\mu_1^{\{\ell_{\mathcal{P}}\}} \doteq \int_0^\infty dy y \mathcal{A}_1^{\{\ell_{\mathcal{P}}\}}(y) \cdot \left( \Psi_1^{\{\ell_{\mathcal{P}}\}}(y) \right)^2. \quad (31)$$

Since we are dealing with an exact solution  $A_1^{\{\ell_{\mathcal{P}}\}}(r)$  (25) of the Poisson equation (24) the Poisson constraint  $\mathbb{N}_G^{[\text{e}]}(12)$  is zero

$$\mathbb{N}_{G,1}^{\{\ell_{\mathcal{P}}\}} \doteq \mathbb{E}_{R,1}^{\{\ell_{\mathcal{P}}\}} - \mathbb{M}_1^{\{\ell_{\mathcal{P}}\}}c^2 \equiv 0 \quad (32)$$

which entails the equality of both coefficients (28) and (31)

$$\varepsilon_{\text{pot},1}^{\{\ell_{\mathcal{P}}\}} \equiv \mu_1^{\{\ell_{\mathcal{P}}\}}. \quad (33)$$

But now that all constituents of the RST energy functional  $\mathbb{E}_{\text{RST}}$ , cf. (8), are explicitly known in terms of the trial parameter  $\beta$ , one can express the energy functional as an ordinary function of that trial parameter  $\beta$ :

$$\mathbb{E}_{\text{RST}} \Rightarrow \mathbb{E}_1^{\{\ell_{\mathcal{P}}\}}(\beta) = \mathbb{E}_{D,1}^{\{\ell_{\mathcal{P}}\}}(\beta) + \mathbb{E}_{R,1}^{\{\ell_{\mathcal{P}}\}}(\beta), \quad (34)$$

which yields by means of the results (23) and (26)

$$\mathbb{E}_1^{\{\ell_{\mathcal{P}}\}}(\beta) = \frac{e^2}{a_B} \left\{ \frac{(2\beta a_B)^2}{4} - (2\beta a_B) \cdot \mu_1^{\{\ell_{\mathcal{P}}\}} \right\}. \quad (35)$$

According to the *principle of minimal energy*, the wanted energy spectrum  $\mathbb{E}_1^{[\ell_{\mathcal{P}}]}$  is obtained by looking for the minimal value of the energy function  $\mathbb{E}_1^{\{\ell_{\mathcal{P}}\}}(\beta)$ :

$$\frac{d\mathbb{E}_1^{\{\ell_{\mathcal{P}}\}}(\beta)}{d\beta} = 0 , \quad (36)$$

which fixes the minimalizing value of  $\beta$  to

$$2\beta a_B = 2\mu_1^{\{\ell_{\mathcal{P}}\}} . \quad (37)$$

Substituting this back in the energy function  $\mathbb{E}_1^{\{\ell_{\mathcal{P}}\}}(\beta)$  (35) yields for the desired spectrum

$$\mathbb{E}_1^{[\ell_{\mathcal{P}}]} = -\frac{e^2}{4a_B} \left(2\mu_1^{\{\ell_{\mathcal{P}}\}}\right)^2 \simeq -6,8029 \cdot \left(2\mu_1^{\{\ell_{\mathcal{P}}\}}\right)^2 , \quad (38)$$

see **table I**.

The most striking element of the precedent results (table I) refers to the groundstate energy ( $n_{\mathcal{P}} = 1 \Leftrightarrow \ell_{\mathcal{P}} = 0$ , first line of table I). Here, the lowest order  $\mathbb{E}_1^{[0]}$  of the RST groundstate prediction *exactly* agrees with its conventional counterpart  $E_{\text{conv}}^{(1)}$  (3):

$$\mathbb{E}_1^{[0]} \equiv E_{\text{conv}}^{(1)} = -\frac{e^2}{4a_B} \simeq -6,8029 \dots [\text{eV}] . \quad (39)$$

Though representing a nice result at first glance, this can actually not be considered a success of RST. Whereas  $E_{\text{conv}}^{(1)}$  is an *exact number* in the conventional theory, the numerically identical RST prediction  $\mathbb{E}_1^{[0]}$  (39) is only the *roughest approximation* within the framework of RST. The conclusion is that the corresponding proper groundstate energy must be lower than the conventional energy  $E_{\text{conv}}^{(1)}$  (3), according to the true spirit of the *principle of minimal energy*! In order to come closer to this proper RST energy we have to put forward “better” trial functions than  $\Phi_1^{\{\ell_{\mathcal{P}}\}}(r)$  (22), i. e. “better” in the sense that, by their use, the non-relativistic RST groundstate prediction will be found *below* the conventional result  $E_{\text{conv}}^{(1)}$ .

This conclusion says that the true RST groundstate energy must be distinctly lower than its conventional counterpart  $E_{\text{conv}}^{(1)} = -6,8029 \dots [\text{eV}]$ ; and this does imply that

the “proper” RST spectrum (in the non-relativistic, electrostatic spherically symmetric approximation) can not agree with its conventional counterpart  $E_{\text{conv}}^{(n)}$  (3). The point here is that the lowest-order RST prediction (39) refers to our special spherically symmetric approximation [4] which naturally must surpass the *true* RST result. Consequently, the claim of agreement of the *proper* RST with the conventional prediction (3) is falsified in the non-relativistic domain.

(notation: the “*true*” RST spectrum refers to the original relativistic RST eigenvalue system in the electrostatic approximation, see equations (IV.5a)-(IV.5d) of ref. [4]. The “proper” RST spectrum refers to the non-relativistic spherically symmetric approximation hereof, see equations(4)-(5) in the present text, or equations (IV.93)-(IV.96) of ref. [4]. This implies that the proper groundstate energy cannot be smaller than the true groundstate energy!)

$n_\varphi (= l_\varphi + 1)$	$\varepsilon_{\text{pot},1}^{\{\ell_{\mathcal{P}}\}}$ (29)	$\mathbb{E}_1^{[\ell_{\mathcal{P}}]}$ [eV] (38)	$E_{\text{conv}}^{(n)}$ (3)	$\frac{E_{\text{conv}}^{(n)} - \mathbb{E}_1^{[\ell_{\mathcal{P}}]}}{E_{\text{conv}}^{(n)}} [\%]$
1	0.500000	−6.802900	−6.802900	0.0
2	0.229167	−1.429081	−1.700725	16.0
3	0.150781	−0.618655	−0.755878	18.2
4	0.112932	−0.347050	−0.425181	18.4
5	0.090503	−0.222886	−0.272116	18.1
6	0.075619	−0.155603	−0.188969	17.7
10	0.045864	−0.057240	−0.068029	15.9
15	0.030886	−0.025958	−0.030235	14.1
20	0.023332	−0.014813	−0.017007	12.9
25	0.018767	−0.009584	−0.010885	11.9
30	0.015707	−0.006713	−0.007559	11.2
35	0.013510	−0.004967	−0.005553	10.6
40	0.011856	−0.003825	−0.004252	10.0
45	0.010565	−0.003037	−0.003359	9.6
50	0.009529	−0.002471	−0.002721	9.2
60	0.007969	−0.001728	−0.001890	8.5
70	0.006850	−0.001277	−0.001388	8.0
80	0.006008	−0.000982	−0.001063	7.6
90	0.005351	−0.000779	−0.000840	7.2
100	0.004824	−0.000633	−0.000680	6.9

**Table I: *Energy Predictions  $\mathbb{E}_1^{[\ell_{\mathcal{P}}]}$  (38) due to the Starting Configuration  $\Phi_1^{\{\ell_{\mathcal{P}}\}}(r)$  (22)***

The energy values  $\mathbb{E}_1^{[\ell_{\mathcal{P}}]}$  (third column) show a deviation of 7% up to 18% from their conventional counterpart  $E_{\text{conv}}^{(n)}$  (3). The average deviation is 12,2%. These lowest-order predictions can be improved considerably by use of better trial functions, see below.

#### 4. *A First Improvement of the Groundstate Energy* ( $\ell_P = 0$ )

In search of a better trial function for the RST groundstate we propose the following (in dimensionless notation):

$$\Psi_\infty^{\{0\}}(y) = \sqrt{\frac{1 - e^{-g}}{g}} \cdot \frac{e^{-y/2}}{1 - (1 - e^{-g}) \cdot e^{-y}} , \quad (40)$$

see **Fig.1**. Here, the constant  $g$  plays the part of the variational parameter; and the normalization condition (15) can be satisfied for all values of this variational parameter, i. e. we actually have

$$1 = \int_0^\infty dy y \left( \Psi_\infty^{\{0\}}(y) \right)^2 . \quad (41)$$

The goal is now to set up the corresponding energy function  $\mathbb{E}_\infty^{\{0\}}(\beta, g)$  as a function of the two variational parameters  $\beta$  and  $g$ :

$$\mathbb{E}_\infty^{\{0\}}(\beta, g) = \mathbb{E}_{D,\infty}^{\{0\}}(\beta, g) + \mathbb{E}_{R,\infty}^{\{0\}}(\beta, g) . \quad (42)$$

Here, both energy contributions, i. e. the matter energy  $\mathbb{E}_{D,\infty}^{\{0\}}$  (14) and the electrostatic field energy  $\mathbb{E}_{R,\infty}^{\{0\}}$  (10), do appear again in the well-known form

$$\mathbb{E}_{D,\infty}^{\{0\}}(\beta, g) = \varepsilon_{\text{kin},\infty}^{\{0\}}(g) \cdot (2\beta a_B)^2 \quad (43a)$$

$$\mathbb{E}_{R,\infty}^{\{0\}}(\beta, g) = -\varepsilon_{\text{pot},\infty}^{\{0\}}(g) \cdot (2\beta a_B) \quad (43b)$$

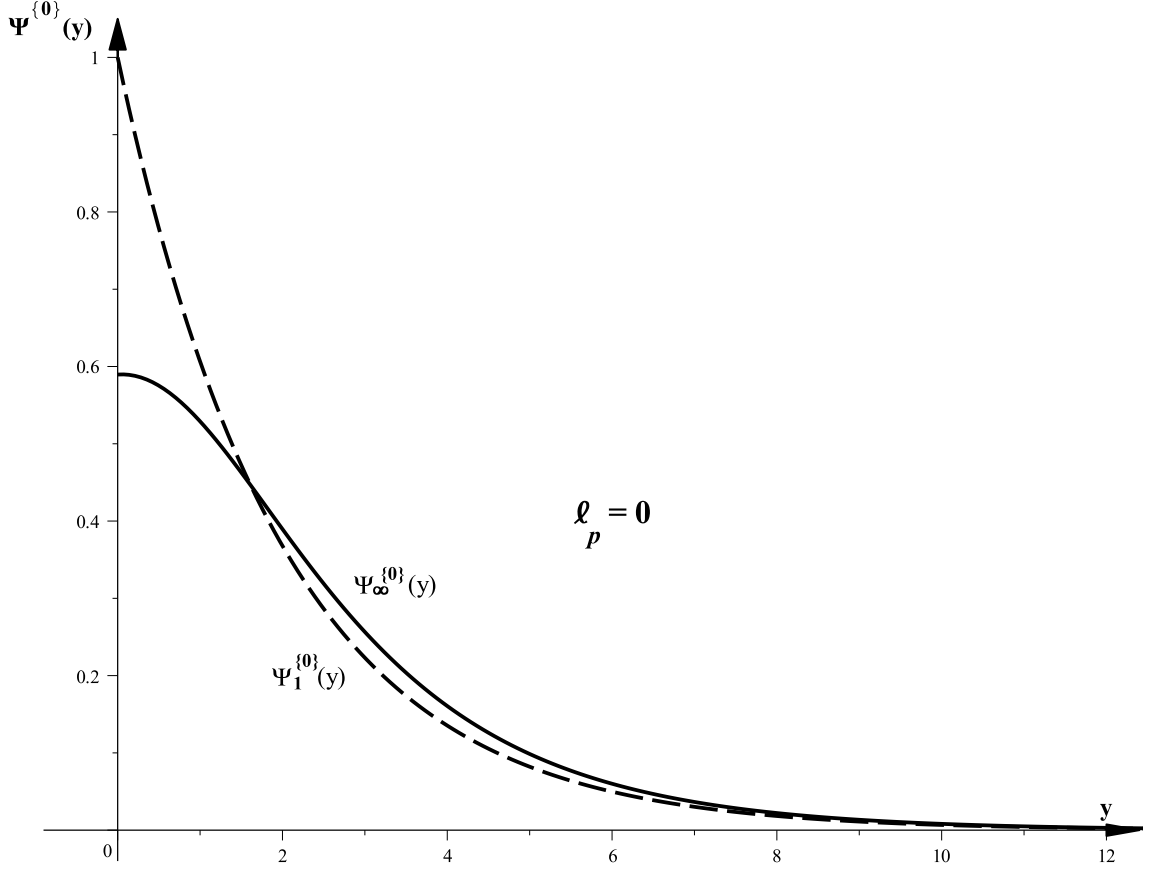
with the kinetic and potential coefficients being defined as usual

$$\varepsilon_{\text{kin},\infty}^{\{0\}}(g) \doteq \int_0^\infty dy y \left( \frac{d \Psi_\infty^{\{0\}}(y)}{dy} \right)^2 \quad (44a)$$

$$\varepsilon_{\text{pot},\infty}^{\{0\}}(g) \doteq \int_0^\infty dy y^2 \left( \frac{d \mathcal{A}_\infty^{\{0\}}(y)}{dy} \right)^2 . \quad (44b)$$

Thus the wanted energy function  $\mathbb{E}_\infty^{\{0\}}(\beta, g)$  is found to appear in the following form:

$$\mathbb{E}_\infty^{\{0\}}(\beta, g) = \frac{e^2}{a_B} \left\{ \varepsilon_{\text{kin},\infty}^{\{0\}}(g) \cdot (2\beta a_B)^2 - \varepsilon_{\text{pot},\infty}^{\{0\}}(g) \cdot (2\beta a_B) \right\} . \quad (45)$$



**Fig.1** *Trial Function  $\Psi_{\infty}^{\{0\}}(y)$  (40) and Lowest-Order Approximation  $\Psi_1^{\{0\}}(y)$  (27c) (broken line)*

The normalized trial function  $\Psi_{\infty}^{\{0\}}(y)$  (40) is shown for the extremalizing value  $g_* = -\ln 2 = -0.69314\dots$ . The corresponding groundstate energy is  $\mathbb{E}_{\infty}^{[0]} \doteq \mathbb{E}_{\infty}^{\{0\}}(g)\Big|_{g=g_*} \simeq -7,6644 [eV]$ , see **Fig. 2**. It is believed that this energy prediction is close to the (unknown) *true* value of the RST groundstate energy. This energy-minimalizing trial function  $\Psi_{\infty}^{\{0\}}(y)$  (40) due to  $g_* = -\ln 2$  has vanishing derivative at the origin

$$\left. \frac{d\Psi_{\infty}^{\{0\}}(y)}{dy} \right|_{y=0} = 0 . \quad (46)$$



In contrast to this, the lowest-order wave function  $\Psi_1^{\{0\}}(y)$  (27c) has a tip at the origin ( $y = 0$ )

$$\left. \frac{d\Psi_1^{\{0\}}(y)}{dy} \right|_{y=0} = -\frac{1}{2}, \quad (47)$$

but it yields (*incidentally*) the exact conventional energy  $E_{\text{conv}}^{(1)}$ , see **table I**.

\*

The stationary points of that energy function (45) over the two-dimensional configuration space, being parameterized by the pair  $(\beta, g)$  of trial parameters, are determined by the usual conditions

$$\left. \frac{\partial \mathbb{E}_\infty^{\{0\}}(\beta, g)}{\partial \beta} \right|_{\beta_*, g_*} = 0 \quad (48a)$$

$$\left. \frac{\partial \mathbb{E}_\infty^{\{0\}}(\beta, g)}{\partial g} \right|_{\beta_*, g_*} = 0, \quad (48b)$$

so that the groundstate energy  $\mathbb{E}_\infty^{[0]}$  is given by

$$\mathbb{E}_\infty^{[0]} \doteq \mathbb{E}_\infty^{\{0\}}(\beta, g) \Big|_{\beta_*, g_*}. \quad (49)$$

But since the energy function  $\mathbb{E}_\infty^{\{0\}}(\beta, g)$  (45) is a simple quadratic function of the first trial parameter  $\beta$ , the first one (48a) of the two extremalization conditions (48a)-(48b) can be written down immediately and yields the extremalizing value of  $\beta$  as

$$2\beta a_B = \frac{\varepsilon_{\text{pot},\infty}^{\{0\}}}{2\varepsilon_{\text{kin},\infty}^{\{0\}}}. \quad (50)$$

This relation may now be used in order to eliminate the first trial parameter  $\beta$  from the energy function  $\mathbb{E}_\infty^{\{0\}}(\beta, g)$  (45) which leaves us with a *one-dimensional* extremalization problem

$$\mathbb{E}_\infty^{\{0\}}(\beta, g) \Rightarrow \mathbb{E}_\infty^{\{0\}}(g) = -\frac{e^2}{4a_B} \frac{\left(\varepsilon_{\text{pot},\infty}^{\{0\}}(g)\right)^2}{\varepsilon_{\text{kin},\infty}^{\{0\}}(g)}. \quad (51)$$

Since both coefficients  $\varepsilon_{\text{pot},\infty}^{\{0\}}$  and  $\varepsilon_{\text{kin},\infty}^{\{0\}}$  depend solely on the second variational parameter  $g$ , the extremalization of the reduced energy function  $\mathbb{E}_{\infty}^{\{0\}}(g)$  (51) may be finally performed by means of an appropriate numerical program.

To this end, one merely has to determine both coefficients  $\varepsilon_{\text{kin},\infty}^{\{0\}}$  and  $\varepsilon_{\text{pot},\infty}^{\{0\}}$  (44a)–(44b) as functions of the second variational parameter  $g$ . For the first one (44a) one finds through the use of our proposed trial ansatz  $\Psi_{\infty}^{\{0\}}(y)$  (40)

$$\varepsilon_{\text{kin},\infty}^{\{0\}} = \frac{g + 2 e^g (e^g - 1)}{12g} . \quad (52)$$

In order to determine the second coefficient  $\varepsilon_{\text{pot},\infty}^{\{0\}}$  (44b), one first has to work out the electrostatic potential  $\mathcal{A}_{\infty}^{\{0\}}(y)$  as solution of the Poisson equation

$$\Delta_y \mathcal{A}_{\infty}^{\{0\}}(y) = - \frac{\left( \Psi_{\infty}^{\{0\}}(y) \right)^2}{y} \quad (53)$$

$$\left( \mathcal{A}_{\infty}^{\{0\}}(y) \div \frac{A_{\infty}^{\{0\}}(r)}{2\beta\alpha_s} \right)$$

which is the dimensionless version of the original Poisson equation (4). The desired solution hereof looks as follows

$$\mathcal{A}_{\infty}^{\{0\}}(y) = \frac{1}{y} \left\{ 1 + \frac{1}{g} \cdot \ln [1 - (1 - e^{-g}) \cdot e^{-y}] \right\} . \quad (54)$$

As a brief check of the boundary conditions one lets  $y$  tend to infinity and finds

$$\lim_{y \rightarrow \infty} \mathcal{A}_{\infty}^{\{0\}}(y) = \frac{1}{y} , \quad (55)$$

i. e. the dimensionless version of the former limit (17). Furthermore, the potential  $\mathcal{A}_{\infty}^{\{0\}}(y)$  (54) assumes a finite value at the origin ( $y = 0$ )

$$\lim_{y \rightarrow 0} \mathcal{A}_{\infty}^{\{0\}}(y) = \frac{e^g - 1}{g} . \quad (56)$$

This can be independently checked by reference to the integral representation of the solution of the Poisson equation (53)

$$\mathcal{A}_{\infty}^{\{0\}}(y) = \frac{1}{4\pi} \int \frac{d^3 \vec{y}'}{y'} \frac{\left( \Psi_{\infty}^{\{0\}}(y') \right)^2}{\|\vec{y} - \vec{y}'\|} , \quad (57)$$

i.e. at the origin  $y \doteq ||\vec{y}|| = 0$

$$\mathcal{A}_{\infty}^{\{0\}}(y) \Big|_{y=0} = \int_0^{\infty} dy' \left( \Psi_{\infty}^{\{0\}}(y') \right)^2 = \frac{e^g - 1}{g} \quad (58)$$

in agreement with the limit (56). Finally, one lets the variational parameter  $g$  in (54) tend to zero and thus finds

$$\lim_{g \rightarrow 0} \mathcal{A}_{\infty}^{\{0\}}(y) = \frac{1 - e^{-y}}{y} \equiv \mathcal{A}_1^{\{0\}}(y) \quad (59)$$

where  $\mathcal{A}_1^{\{0\}}(y)$  (27b) is nothing else than the dimensionless version of  $A_1^{\{0\}}(r)$  (25). This result meets with the expectation for the limit  $g \rightarrow 0$ , because in this limit our ansatz  $\Psi_{\infty}^{\{0\}}(y)$  (40) tends to the former simplest trial function  $\Psi_1^{\{0\}}(y)$  (27c)

$$\lim_{g \rightarrow 0} \Psi_{\infty}^{\{0\}}(y) = \Psi_1^{\{0\}}(y) , \quad (60)$$

and the corresponding potential  $A_1^{\{0\}}(r)$  (25) as solution of the Poisson equation (24) for  $\ell_{\mathcal{P}} = 0$  reads in the dimensionless notation as expected

$$\mathcal{A}_1^{\{0\}}(y) = \frac{1 - e^{-y}}{y} , \quad (61)$$

cf. (59).

But now that the potential  $\mathcal{A}_{\infty}^{\{0\}}(y)$  is explicitly known, cf. (54), one can substitute this in the equation (44b) in order to determine the potential coefficient  $\varepsilon_{\text{pot},\infty}^{\{0\}}$  as a function of the variational parameter  $g$ . Alternatively, one could substitute also both fields  $\Psi_{\infty}^{\{0\}}(y)$  and the associated potential  $\mathcal{A}_{\infty}^{\{0\}}(y)$  in the mass equivalent, cf. (30)

$$\mathbb{M}_{\infty}^{\{0\}} c^2 = - \frac{e^2}{a_B} (2\beta a_B) \cdot \mu_{\infty}^{\{0\}}(g) \quad (62a)$$

$$\mu_{\infty}^{\{0\}}(g) \doteq \int_0^{\infty} dy \, y \, \mathcal{A}_{\infty}^{\{0\}}(y) \left( \Psi_{\infty}^{\{0\}}(y) \right)^2 \quad (62b)$$

and must then obtain as a check the Poisson constraint in coefficient form

$$\varepsilon_{\infty}^{\{0\}}(g) \equiv \mu_{\infty}^{\{0\}}(g) . \quad (63)$$

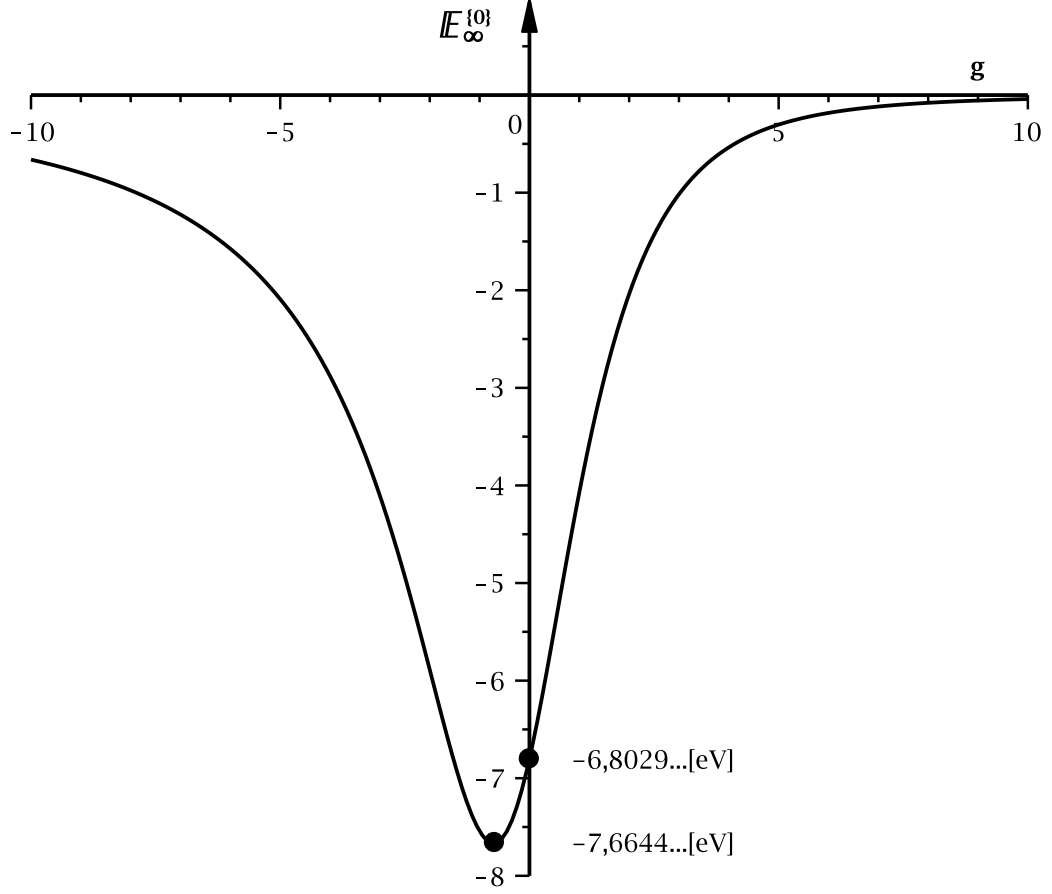
The result is

$$\varepsilon_{\text{pot},\infty}^{\{0\}}(g) \equiv \mu_{\infty}^{\{0\}}(g) = \frac{e^g - (1 + g)}{g^2} . \quad (64)$$

With both coefficients  $\varepsilon_{\text{kin},\infty}^{\{0\}}$  and  $\varepsilon_{\text{pot},\infty}^{\{0\}}$  being now explicitly known as functions of the solely remaining parameter  $g$ , one can substitute these results in the reduced energy function  $\mathbb{E}_{\infty}^{\{0\}}(g)$  (51) which thereby adopts the following shape

$$\mathbb{E}_{\infty}^{\{0\}}(g) = -\frac{e^2}{4a_B} \frac{12}{g^3} \frac{[e^g - (1 + g)]^2}{g + 2 e^g (e^g - 1)} . \quad (65)$$

The groundstate energy  $\mathbb{E}_{\infty}^{[0]} = -7,6644 \dots$  [eV] is found as the minimal value of this energy function by means of a suitable numerical program, see **Fig.2**. The energy-minimalizing value of  $g$  is found as  $g_* = -\ln 2 = -0,69314 \dots$  which however can also be determined from the requirement that our trial ansatz  $\Psi_{\infty}^{\{0\}}(y)$  (40) have vanishing derivative on the origin ( $y = 0$ ), see **Fig.1**. Such a requirement may be philosophically justified through the viewpoint that nature dislikes singularities but prefers smooth functions.



**Fig.2** *Energy Function*  $\mathbb{E}_{\infty}^{\{0\}}(g)$  (65)

The groundstate energy  $\mathbb{E}_{\infty}^{[0]} = -7,6644\dots[\text{eV}]$ , due to the ansatz  $\Psi_{\infty}^{\{0\}}(y)$  (40), is the minimal value of the energy function  $\mathbb{E}_{\infty}^{\{0\}}(g)$  (65), occurring for  $g_* = -\ln 2 = -0.69314\dots$ , cf. (46), and thus is distinctly lower than the conventional prediction  $\mathbb{E}_{\text{conv}}^{(1)} = -6,8029\dots[\text{eV}]$ , cf. (3). The energy curve  $\mathbb{E}_{\infty}^{\{0\}}(g)$  intersects the energy axis ( $g = 0$ ) at the conventional value  $\mathbb{E}_{\text{conv}}^{(1)}$  (3) because our extended ansatz  $\Psi_{\infty}^{\{0\}}(y)$  (40) becomes reduced to the lowest-order approximation  $\Psi_1^{\{0\}}(y)$  (27c) for  $g \rightarrow 0$ . Incidentally, the corresponding lowest-order groundstate energy  $\mathbb{E}_1^{[0]}$  (39) is identical to the conventional energy  $E_{\text{conv}}^{(1)} = -6,8029[\text{eV}]$ , see **table I**.

Besides by means of a numerical program, the minimal value  $\mathbb{E}_\infty^{[0]}$  (49) can also be found by a more intuitive guess: Namely, the set of trial ansätze  $\Psi_\infty^{\{0\}}(y)$  (40) with variational parameter  $g$  contains a member ( $\overset{\circ}{\Psi}_\infty^{\{0\}}(y)$ , say) which has vanishing derivative at the origin

$$\frac{d\overset{\circ}{\Psi}_\infty^{\{0\}}(y)}{dy} = 0 . \quad (66)$$

This specific member is characterized through a special value ( $g_*$ ) of the variational parameter  $g$

$$g \Rightarrow g_* = -\ln 2 = -0,69314 . \quad (67)$$

For this situation (67), the general trial ansatz  $\Psi_\infty^{\{0\}}(y)$  (40) adopts the special form

$$\Psi_\infty^{\{0\}}(y) \Rightarrow \overset{\circ}{\Psi}_\infty^{\{0\}}(y) = \frac{1}{2\sqrt{\ln 2}} \cdot \frac{1}{\cosh \frac{y}{2}} . \quad (68)$$

Of course, this wave function  $\overset{\circ}{\Psi}_\infty^{\{0\}}(y)$  is normalized to unity

$$\int_0^\infty dy y \left( \overset{\circ}{\Psi}_\infty^{\{0\}}(y) \right)^2 = 1 \quad (69)$$

since the normalization condition (41) is satisfied by *all* members of the trial set  $\Psi_\infty^{\{0\}}(y)$  (40).

Concerning now the energy ( $\overset{\circ}{\mathbb{E}}_\infty^{[0]}$ , say) due to the present groundstate ansatz  $\overset{\circ}{\Psi}_\infty^{\{0\}}(y)$  (68), it should be clear that the energy function  $\mathbb{E}_\infty^{\{0\}}(g)$  (51) assumes its minimal value  $\overset{\circ}{\mathbb{E}}_\infty^{[0]}$  at  $g_*$  (67)

$$\overset{\circ}{\mathbb{E}}_\infty^{\{0\}}(g_*) \doteq \overset{\circ}{\mathbb{E}}_\infty^{[0]} = -\frac{e^2}{4a_B} \frac{\left( \overset{\circ}{\varepsilon}_{\text{pot},\infty}^{\{0\}} \right)^2}{\overset{\circ}{\varepsilon}_{\text{kin},\infty}^{\{0\}}} . \quad (70)$$

Here the electrostatic coefficient  $\overset{\circ}{\varepsilon}_{\text{pot},\infty}^{\{0\}}$  is to be deduced from its general form (44b) as

$$\varepsilon_{\text{pot},\infty}^{\{0\}} \Rightarrow \overset{\circ}{\varepsilon}_{\text{pot},\infty}^{\{0\}} = \int_0^\infty dy y^2 \left( \frac{d\overset{\circ}{\mathcal{A}}_\infty^{\{0\}}(y)}{dy} \right)^2 , \quad (71)$$

and similarly the kinetic coefficient  $\overset{\circ}{\varepsilon}_{\text{kin},\infty}^{\{0\}}$  is a specialization of  $\varepsilon_{\text{kin},\infty}^{\{0\}}$  (44a):

$$\varepsilon_{\text{kin},\infty}^{\{0\}} \Rightarrow \overset{\circ}{\varepsilon}_{\text{kin},\infty}^{\{0\}} = \int_0^\infty dy y \left( \frac{d\overset{\circ}{\Psi}_\infty^{\{0\}}(y)}{dy} \right)^2 . \quad (72)$$

Thus, one substitutes that special value  $g_*$  (67) in the result (52) for  $\varepsilon_{\text{kin},\infty}^{\{0\}}$  and obtains

$$\varepsilon_{\text{kin},\infty}^{\{0\}} = \frac{\ln 2 + \frac{1}{2}}{12 \ln 2} = 0.14344 \dots \quad (73)$$

In a quite similar way, one obtains also the value of the electrostatic coefficient  $\varepsilon_{\text{pot},\infty}^{\{0\}}$  (71), namely by substituting the special value  $g_*$  in equation (64) which yields

$$\varepsilon_{\text{pot},\infty}^{\{0\}} = \frac{\frac{1}{2} - (1 - \ln 2)}{(\ln 2)^2} = 0.40200 \dots \quad (74)$$

Consequently, the final result (70) is

$$\mathbb{E}_{\infty}^{[0]} \simeq -\frac{e^2}{4a_{\text{B}}} \cdot \frac{(0,40200)^2}{0,14344} = -\frac{e^2}{4a_{\text{B}}} \cdot 1,12663 = -7,6644 [\text{eV}] . \quad (75)$$

Recall here that the RST principle of minimal energy establishes a possibility of ranking the various trial ansätze in the sense that the ansatz with the lower groundstate energy is the better one. In this sense, the present ansatz  $\hat{\Psi}_{\infty}^{\{0\}}(y)$  (68) supercedes all the precedent ansätze of the former papers [4] which predicted a higher groundstate energy. The next step must now refer to the calculation of the excitation spectrum ( $\ell_{\mathcal{P}} \geq 1$ ) by proposing an adequate generalization of the present groundstate ansatz (68).

## 5. *First Improvement for the Excited States* ( $\ell_{\mathcal{P}} \geq 1$ )

We shall now show that a *taller* wave function yields a considerable improvement of the RST energy predictions so that the average deviation (from the conventional predictions) shrinks to (roughly) 3/4 of the zero-order predictions of **table I**. This result says that we have to shape the wave function even taller in order to get that further improvement of our RST energy predictions. For this purpose, we consider now the normalized trial ansatz  $\hat{\Phi}_1^{\{\nu\}}(r)$

$$\hat{\Phi}_1^{\{\nu\}}(r) = \frac{(2\beta)^{\nu+1}}{\sqrt{\Gamma(2\nu+2)}} \cdot r^{\nu} e^{-\beta r} , \quad (76)$$

or rewritten in the dimensionless notation of (27a), (27c):

$$\hat{\Psi}_1^{\{\nu\}}(y) \doteq \frac{\hat{\Phi}_1^{\{\nu\}}(r)}{2\beta} = \frac{y^{\nu}}{\sqrt{\Gamma(2\nu+2)}} \cdot e^{-y/2} . \quad (77)$$

The latter proposition evidently shows that this is effectively a one-parameter trial ansatz with the real-valued variational parameter  $\nu$ . Our general procedure means that we first have to set up the corresponding energy function  $\widehat{\mathbb{E}}_1^{\{\ell_{\mathcal{P}}\}}(\nu)$  as a function of the variational parameter  $\nu$

$$\widehat{\mathbb{E}}_1^{\{\ell_{\mathcal{P}}\}}(\nu) = -\frac{e^2}{4a_B} \frac{\left(\widehat{\varepsilon}_{\text{pot},1}(\nu)\right)^2}{\widehat{\varepsilon}_{\text{kin},1}^{\{\ell_{\mathcal{P}}\}}(\nu)}, \quad (78)$$

and the minimal values  $\mathbb{E}_1^{[\ell_{\mathcal{P}}]}$  of this energy function do then constitute the wanted energy spectrum:

$$\widehat{\mathbb{E}}_1^{[\ell_{\mathcal{P}}]} = \widehat{\mathbb{E}}_1^{\{\ell_{\mathcal{P}}\}}(\nu) \Big|_{\nu=\nu_*}. \quad (79)$$

The energy-minimalizing values  $\nu_*^{[\ell_{\mathcal{P}}]}$  for any quantum number  $\ell_{\mathcal{P}}$  are defined as usual, cf. (48a)-(48b)

$$\frac{d \widehat{\mathbb{E}}_1^{\{\ell_{\mathcal{P}}\}}(\nu)}{d\nu} \Big|_{\nu=\nu_*} = 0. \quad (80)$$

Thus, we are left with the problem of determining the potential coefficient  $\widehat{\varepsilon}_{\text{pot},1}(\nu)$  and the kinetic coefficient  $\widehat{\varepsilon}_{\text{kin},1}^{\{\ell_{\mathcal{P}}\}}(\nu)$  as functions of the variational parameter  $\nu$ .

Observe here that if we replace the variational parameter  $\nu$  in the extended ansatz  $\widehat{\Psi}_1^{\{\nu\}}(y)$  (77) by the quantum number  $\ell_{\mathcal{P}}$  ( $= 1, 2, 3, \dots$ ), then this ansatz becomes reduced to our starting ansatz  $\Psi_1^{\{\ell_{\mathcal{P}}\}}(y)$  (27c) which generates the former **table I**. So we see that our present more general ansatz  $\widehat{\Psi}_1^{\{\nu\}}(y)$  (77) works as a one-dimensional embedding manifold for that most naïve ansatz  $\Psi_1^{\{\ell_{\mathcal{P}}\}}(y)$  (27c). Of course, one expects that the extended set of two-parametric wave functions  $\widehat{\Psi}_1^{\{\nu\}}(y)$  (77) includes for any  $\ell_{\mathcal{P}}$  a member  $\widehat{\Psi}_1^{\{\nu_*\}}(y)$  (off the one-parametric subset  $\Psi_1^{\{\ell_{\mathcal{P}}\}}(y)$ ) which has lower energy  $\widehat{\mathbb{E}}_1^{[\ell_{\mathcal{P}}]}$  (79) than  $\mathbb{E}_1^{[\ell_{\mathcal{P}}]}$  due to the starting ansatz  $\Psi_1^{\{\ell_{\mathcal{P}}\}}(y)$  (27c), cf. **table I** and **table II** below.

Thus the task is now to determine the energy function  $\widehat{\mathbb{E}}_1^{\{\ell_{\mathcal{P}}\}}(\nu)$  (78) as an explicit function of the second variational parameter  $\nu$  (the first parameter  $\beta$  is already eliminated).



Turning here first to the kinetic coefficient  $\widehat{\varepsilon}_{\text{kin},1}^{\{\ell_{\mathcal{P}}\}}(\nu)$

$$\widehat{\varepsilon}_{\text{kin},1}^{\{\ell_{\mathcal{P}}\}}(\nu) \doteq \int_0^\infty dy y \left\{ \left( \frac{d \widehat{\Psi}_1^{\{\nu\}}(y)}{dy} \right)^2 + \ell_{\mathcal{P}}^2 \left( \frac{\widehat{\Psi}_1^{\{\nu\}}(y)}{y} \right)^2 \right\}, \quad (81)$$

and substituting herein our extended ansatz  $\widehat{\Psi}_1^{\{\nu\}}(y)$  (77) yields

$$\widehat{\varepsilon}_{\text{kin},1}^{\{\ell_{\mathcal{P}}\}}(\nu) = \frac{1}{2\nu+1} \left( \frac{1}{4} + \frac{\ell_{\mathcal{P}}^2}{2\nu} \right). \quad (82)$$

Of course, the identification of the real number  $\nu$  with the integer-valued quantum number  $\ell_{\mathcal{P}}$  leads us back to the former result  $\varepsilon_{\text{kin},1}^{\{\ell_{\mathcal{P}}\}} = 1/4$ , cf. (23).

Next, one considers the numerator of the energy  $\widehat{\mathbb{E}}_1^{\{\ell_{\mathcal{P}}\}}(\nu)$  (78), i.e.  $\widehat{\varepsilon}_{\text{pot},1}(\nu) \equiv \widehat{\mu}_1(\nu)$ , with the mass-equivalent coefficient  $\widehat{\mu}_1(\nu)$  being defined as usual, cf. (31)

$$\widehat{\mu}_1(\nu) = \int_0^\infty dy y \widehat{\mathcal{A}}_1^{\{\nu\}}(y) \cdot \left( \widehat{\Psi}_1^{\{\nu\}}(y) \right)^2. \quad (83)$$

Evidently, before being able to calculate this coefficient, we first have to determine the potential  $\widehat{\mathcal{A}}_1^{\{\nu\}}(y)$  from the corresponding Poisson equation, cf. (24)

$$\Delta_y \widehat{\mathcal{A}}_1^{\{\nu\}}(y) = - \frac{\left( \widehat{\Psi}_1^{\{\nu\}}(y) \right)^2}{y}. \quad (84)$$

This reads by explicit reference to the ansatz  $\widehat{\Psi}_1^{\{\nu\}}(y)$  (77)

$$\Delta_y \widehat{\mathcal{A}}_1^{\{\nu\}}(y) = - \frac{y^{2\nu-1}}{\Gamma(2\nu+2)} e^{-y} \quad (85)$$

which however is nothing else than the “continuous” generalization ( $\ell_{\mathcal{P}} \Rightarrow \nu$ ) of the “discrete” equation (24). The solution of that “discrete” Poisson equation (24) is given by equation (25) and the problem is now to transcribe this solution  $\mathcal{A}_1^{\{\ell_{\mathcal{P}}\}}(y)$  from the integer-valued quantum number  $\ell_{\mathcal{P}}$  ( $= 1, 2, 3, 4, \dots$ ) to the real-valued variational parameter  $\nu$ . This may be done by means of some simple mathematical manipulations and the result is

$$\widehat{\mathcal{A}}_1^{\{\nu\}}(y) = \frac{1}{2\nu+1} \left\{ 1 - e^{-y} \sum_{n=0}^{\infty} \frac{n}{\Gamma(2\nu+2+n)} y^{2\nu+n} \right\}. \quad (86)$$

For a quick check of this result one compares it to its integral representation

$$\widehat{\mathcal{A}}_1^{\{\nu\}}(y) = \frac{1}{4\pi\Gamma(2\nu+2)} \int d^3 \vec{y}' \frac{(y')^{2\nu-1} e^{-y'}}{|\vec{y} - \vec{y}'|} \quad (87)$$

which surely satisfies the Poisson equation (85) and has also the required Coulomb form at infinity ( $y \rightarrow \infty$ )

$$\lim_{y \rightarrow \infty} \widehat{\mathcal{A}}_1^{\{\nu\}}(y) = \frac{1}{4\pi\Gamma(2\nu+2)} \cdot \frac{1}{y} \cdot \int d^3 \vec{y}' y'^{2\nu-1} e^{-y'} = \frac{1}{y}, \quad (88)$$

namely just on account of the normalization condition on our generalized trial amplitude  $\widehat{\Psi}_1^{\{\nu\}}(y)$  (77):

$$1 \stackrel{!}{=} \int_0^\infty dy y \left( \widehat{\Psi}_1^{\{\nu\}}(y) \right)^2 = \int_0^\infty dy \frac{y^{2\nu+1} e^{-y}}{\Gamma(2\nu+2)}. \quad (89)$$

On the other hand, the value of this potential  $\widehat{\mathcal{A}}_1^{\{\nu\}}(y)$  at the origin ( $y = 0$ ) can immediately be read off also from its integral representation (87)

$$\widehat{\mathcal{A}}_1^{\{\nu\}}(0) = \frac{1}{\Gamma(2\nu+2)} \int_0^\infty dy y^{2\nu} e^{-y} = \frac{1}{2\nu+1}, \quad (90)$$

which is in agreement with what follows from equation (86). Now when the boundary conditions at the origin and at infinity are the same in both cases (86) and (87) and both forms (86) and (87) do satisfy the Poisson equation (85), they necessarily must be identical; and the solution (86) is what we are after. Indeed, one can also show by straightforward differentiation, that the claimed potential  $\widehat{\mathcal{A}}_1^{\{\nu\}}(y)$  (86) does actually solve the Poisson equation (85).

But now that we have the desired potential at hand we can tackle the problem of the mass-equivalent coefficient  $\widehat{\mu}_1(\nu)$  (83). Inserting here both the potential  $\widehat{\mathcal{A}}_1^{\{\nu\}}(y)$  and the wave function  $\widehat{\Psi}_1^{\{\nu\}}(y)$  (77) yields by means of straightforward integration

$$\begin{aligned} \widehat{\mu}_1(\nu) &= \frac{1}{2\nu+1} \left\{ 1 - \frac{1}{\Gamma(2\nu+2)} \frac{1}{2^{4\nu+2}} \sum_{n=0}^\infty \frac{n}{2^n} \cdot \frac{\Gamma(4\nu+2+n)}{\Gamma(2\nu+2+n)} \right\} \\ &\equiv \frac{1}{2\nu+1} \left\{ 1 - \frac{\Gamma(2\nu+\frac{3}{2})}{\sqrt{\pi} \cdot \Gamma(2\nu+2)} \right\}. \end{aligned} \quad (91)$$

Thus, observing the numerical identity of both coefficients  $\widehat{\varepsilon}_{\text{pot},1}^{\{\nu\}}$  and  $\widehat{\mu}_4^{\{\nu\}}$ , the wanted energy function  $\widehat{\mathbb{E}}_1^{\{\ell_{\mathcal{P}}\}}(\nu)$  (78) is completely determined as a function of the variational parameter  $\nu$ ; and one can determine the energy spectrum  $\widehat{\mathbb{E}}_1^{[\ell_{\mathcal{P}}]}$  (79) through the recipe (79)-(80), see **table II** below.

The results of **table II**, being due to the ansatz  $\widehat{\Psi}_1^{\{\nu\}}(y)$  (77), show two details being worth while in order to be considered. Firstly, the groundstate energy  $\widehat{\mathbb{E}}_1^{[0]}(\rightsquigarrow n_{\mathcal{P}} = 1 \Leftrightarrow \ell_{\mathcal{P}} = 0, \text{ first line})$  is lowered down to  $-7,2311 \dots$  [eV] below the conventional value of  $-6,8029 \dots$  [eV] which is due to the conventional prediction (3). But this is still above the groundstate prediction of  $-7,6644 \dots$  [eV] due to the “infinite” ansatz  $\overset{\circ}{\Psi}_{\infty}^{\{0\}}(y)$  (68), see **Fig.2**. This might be considered a hint at the possibility that the *exact* RST predictions for  $\ell_{\mathcal{P}} \geq 1$  are also *below* their conventional counterparts  $\mathbb{E}_{\text{conv}}^{(n)}$  (3), *not above* them as could be concluded from the precedent **table I** and subsequent **table II**. Therefore one furthermore has to look for better trial functions in order to decide this question.

Secondly, the *average deviation* for  $1 \leq \ell_{\mathcal{P}} \leq 100$  (last column of **table II**) receives now a considerable improvement relative to the precedent results of **table I**: we have here now 7,8% deviation in place of 12,2% there. This endows our present ansatz (77) with a better predictive quality than its predecessor  $\Psi_1^{\{\ell_{\mathcal{P}}\}}(y)$  (27c) ( $\Rightarrow$  **table I**).

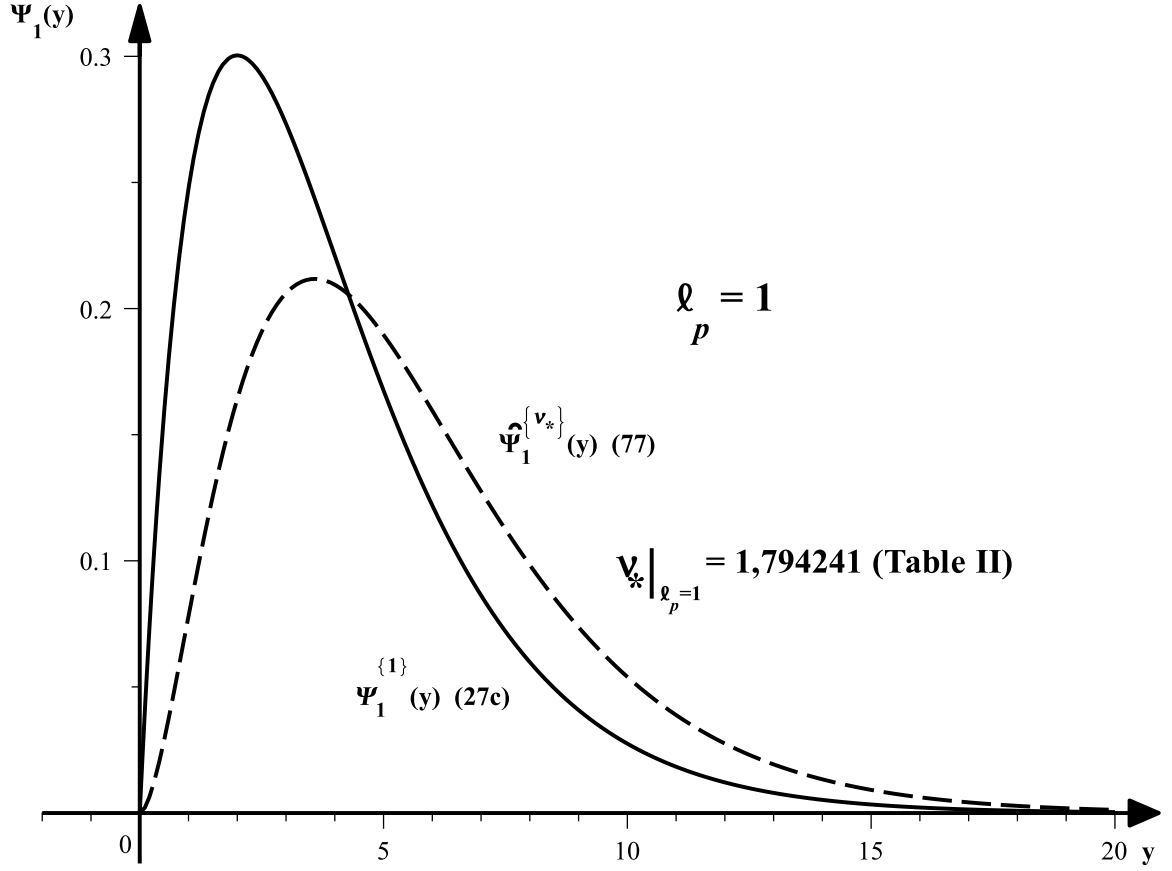
$n_{\mathcal{P}} (= \ell_{\mathcal{P}} + 1)$	$\mathbb{E}_{\text{conv}}^{(n)} [\text{eV}], (3)$	$\widehat{\mathbb{E}}_1^{[\ell_{\mathcal{P}}]} [\text{eV}], (79)$	$\nu_*(80)$	$2\beta_* a_B$	$\frac{E_{\text{conv}}^{(n)} - \widehat{\mathbb{E}}_1^{[\ell_{\mathcal{P}}]}}{E_{\text{conv}}^{(n)}} [\%]$
1	-6.802900	-7.231189	-0.204907	0.792050	-6.30
2	-1.700725	-1.551005	1.794241	0.703351	8.8
3	-0.755878	-0.669200	3.752794	0.516880	11.5
4	-0.425181	-0.373694	5.87049	0.415087	12.1
5	-0.272116	-0.239081	8.130662	0.350581	12.1
6	-0.188969	-0.166388	10.504450	0.305707	11.9
10	-0.068029	-0.060694	20.953757	0.209389	10.8
15	-0.030235	-0.027356	35.701713	0.155896	9.5
20	-0.017007	-0.015549	51.919571	0.126789	8.6
25	-0.010885	-0.010030	69.357145	0.108158	7.8
30	-0.007559	-0.007009	87.851123	0.095065	7.3
35	-0.005553	-0.005176	107.284631	0.085285	6.8
40	-0.004252	-0.003980	127.568998	0.077660	6.4
45	-0.003359	-0.003156	148.634158	0.071521	6.1
50	-0.002721	-0.002564	170.423058	0.066456	5.8
60	-0.001890	-0.001790	215.989099	0.058550	5.3
70	-0.001388	-0.001320	263.963879	0.052624	4.9
80	-0.001063	-0.001014	314.117619	0.047992	4.6
90	-0.000840	-0.000804	366.268979	0.044254	4.3
100	-0.000680	-0.000653	420.270468	0.041164	4.1

**Table II: *Extremal Values*  $\widehat{\mathbb{E}}_1^{[\ell_{\mathcal{P}}]}$  (79) of the Energy Function  $\widehat{\mathbb{E}}_1^{\{\ell_{\mathcal{P}}\}}(\nu)$  (78)**

The extremal values  $\widehat{\mathbb{E}}_1^{[\ell_{\mathcal{P}}]}$  (79) of the energy function  $\widehat{\mathbb{E}}_1^{\{\ell_{\mathcal{P}}\}}(\nu)$  (78) occur at the extremalizing values  $\nu_*$  and  $\beta_*$  and are given by

$$\widehat{\mathbb{E}}_1^{\{\ell_{\mathcal{P}}\}} = -\frac{e^2}{4a_B} \cdot \frac{\widehat{\varepsilon}_{\text{pot},1}^2(\nu_*)}{\widehat{\varepsilon}_{\text{kin},1}^{\{\ell_{\mathcal{P}}\}}(\nu_*)} = -\frac{e^2}{4a_B} \cdot \frac{(4\beta_* a_B)^2}{2\nu_* + 1} \left( \frac{1}{4} + \frac{\ell_{\mathcal{P}}^2}{2\nu_*} \right). \quad (92)$$

The improvement from an average deviation of 12,2% (**table I**) to 7,8% (table II) raises the question through what deformation of the trial function such an improvement could be obtained. The answer comes from a comparison of the zero-order function  $\Psi_1^{\{\ell_{\mathcal{P}}\}}(y)$  (27c) ( $\rightsquigarrow$  **table I**) to the firstly improved function  $\widehat{\Psi}_1^{\{\nu\}}(y)$  (77); see **Fig.3** below, for  $\ell_{\mathcal{P}} = 1$ . Evidently, the better trial function  $\widehat{\Psi}_1^{\{\nu\}}(y)$  for the optimal value  $\nu_*$  of the parameter  $\nu$  (i.e.  $\nu_*|_{\ell_{\mathcal{P}}=1} = 1,794241$ , see **table II**) is less concentrated (localized) around its maximum (at  $y_* = 3,5884\dots$ ). This delocalization effect is responsible for the fact that the energy  $\widehat{\mathbb{E}}_1^{[\ell_{\mathcal{P}}]}$  due to  $\widehat{\Psi}_1^{\{\nu_*\}}(y)$  matches better with the conventional prediction  $E_{\text{conv}}^{(1)}$  (3): the deviation for  $\Psi_1^{\{1\}}(y)$  (27c) is 16% (**table I**) whereas for the present  $\widehat{\Psi}_1^{\{\nu_*\}}(y)$  (77) one has now a deviation of only 8,8%.



**Fig.3** *Improvement of the Energy Predictions through Delocalization ( $\ell_p = 1$ )*

Through broadening the zero-order trial function  $\Psi_1^{\{\ell_p\}}(y)$  (27c) to the firstly improved function  $\hat{\Psi}_1^{\{\nu\}}(y)$  (77) one gets a corresponding improvement of the energy prediction from 16% deviation (**table I**, second line) to only 8,8% deviation (**table II**, second line). This is a similar effect as for the groundstate ( $\ell_p = 0$ ), **Fig. 1**, where the more delocalized function  $\Psi_\infty^{\{0\}}(y)$  (40) entails a lowering of the energy prediction from  $\mathbb{E}_1^{[0]} = -6,8029 \text{ [eV]}$  (39) to  $\mathbb{E}_\infty^{[0]} = -7,6644 \text{ [eV]}$ , see **Fig.2**.

## Summary

An approximate groundstate energy  $\mathbb{E}_{\infty}^{[0]}$  has been found by means of a variational method in the range of  $-7,6644$  [eV] as compared to the conventional value of  $E_{\text{conv}}^{(1)} = -6,8029$  [eV], see **Fig.2**. Concerning the whole energy spectrum (up to quantum numbers  $\rightsquigarrow 100$ ), the simpler trial ansatz  $\widehat{\Psi}_1^{\{\nu\}}(y)$  (77) yielded energy predictions with an average deviation of 9% from the conventional values  $E_{\text{conv}}^{(n)}$  (3). The underlying approximation assumption refers to the *spherically symmetric approximation* (ref. [4], equations (IV.6a)-(IV.7b)). From the fact that the corresponding energy predictions are relatively close to the conventional values  $E_{\text{conv}}^{(n)}$  (3), except for the groundstate, one may conclude that the *exact* RST predictions could possibly lie in an even more narrow neighborhood of their conventional counterparts. Such a result would be necessary in order that RST can be considered a serious competitor of the conventional theory.

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$$\ell_p = 1$$

